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Inversion of Structural Dynamics Simulations: State-of-the-art and Orientations of the Research[1]

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Abstract

This publication offers an overview of the technology available for formulating inverse problems and correlating measured responses with simulations from finite element analysis. The application targeted is clearly structural dynamics although most of the techniques discussed here originate or find their counterparts in physics and other engineering fields. After reviewing the state-of-the-art practices in model updating where a mostly linear model is optimized to satisfy a series of modal criteria of correlation, an assessment of the advantages and limitations of this technology is offered. Current orientations of inverse problem solving are discussed, including the need to propagate variability through the simulation; the generation of fast running models; the adequate choice of data metrics for nonlinear dynamics; sampling strategies for the optimization; and hypothesis testing in the context of multivariate data analysis.

1. Introduction

Inverse problem solving is at the core of engineering practices as such work generally involves designing a system to target a given performance or to satisfy operating constraints. Increasingly, designers are faced with shorter design cycles while their testing capabilities are reduced and the physics they must understand becomes more sophisticated. The consequence is the need for new, component-level testing procedures, larger-size computer models, coupled-field calculations and more accurate representations of the physics. To improve the predictive quality of numerical models and enhance the capability to extrapolate the response of a system, it is often necessary to formulate and solve inverse problems where simulations are compared to field measurements [1].

In the field of structural dynamics, computational models are developed for predicting the response of a system when the phenomenon is not accessible by direct measurement or when numerical simulations are cheaper than testing. To develop high-fidelity models, analysts are increasingly obliged to account for nonlinearity and variability. These two aspects are particularly emphasized throughout this publication. In the first case, material nonlinearity (such as hardening) may be required to represent the behavior of structural components; geometrical nonlinearity may result from large displacement and/or large deformation motions; and the loading applied may excite the response's spectral content in the high-frequency range, making it more important to account for nonlinearity and damping properties. In the second case, it is acknowledged that some design variables are randomly distributed (for example, the thickness distribution of a shell after a press-forming process) or that the environment influences significantly the system. To provide high-fidelity models, these variations must be propagated throughout the calculation. Nevertheless, implementing sophisticated models does not necessarily provide a more accurate representation of a system. After developing a model, it must be verified that the discretization, mathematical idealization and other assumptions involved yield a satisfactory solution. Capturing "rare" or catastrophic events occurring at the tails of the probabilistic distributions involved is also of paramount importance for reliability analysis and safety assessment. This is known as model validation and it is usually carried out by comparing the prediction of a model or family of models to test data. If the agreement between the two sets is not satisfactory, design parameters can be optimized to improve the predictive quality of the models.

The work presented in this publication addresses the general problem of validating numerical models in the context of nonlinear structural dynamics, stochastic simulations and transient excitation. We start by discussing current trends in computational sciences (Section 3) and structural dynamics (Section 4). The publication proceeds in Section 5 with a brief presentation of the concept of Finite Element (FE) model updating because it generally constitutes the starting point of model validation for nonlinear dynamics. The broader concept of model validation is

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presented in Section 6 and several research directions are discussed to illustrate the shift of paradigm that, we believe, will be necessary to solve inverse, test-analysis correlation problems for nonlinear and stochastic structural dynamics.

2. Scope of the Discussion

Our perspective is strongly influenced by many discussions with experimentalists, analysts, structural dynamicists, climatologists, physicists and statisticians from LANL and Sandia National Laboratories (SNL). Therefore, the point of view presented here will be more representative of the U.S. and its national laboratories. At the national laboratories, the corner stone of the research in model validation is the U.S. Department of Energy's Accelerated Strategic Computing Initiative (ASCI), a program that is developing massively parallel hardware and software environments for enhancing the modeling, predictive quality and reliability of computer simulations for non-conventional, defense applications. Hence, our "philosophy" of model validation is geared towards making use of these resources and satisfying the constraints associated with the ASCI environment and the applications specific to LANL. Nevertheless, we believe that our findings are general enough that they may be relevant to many other technical communities and environments. For completeness, the reader is referred to the work of Worden who presents an European perspective of similar issues [2].

3. Computational Sciences

Current trends in computational sciences are briefly discussed. The intent is to show that trends that can currently be observed in structural dynamics are not specific to this community. Also, we would like to promote the idea that experience may be gained from learning what is being achieved in other scientific communities.

3.1 What Model for What Purpose?

The dynamics of systems commonly analyzed in most computational sciences is strongly influenced by the nature of particular partial differential equations. When complex phenomena are studied, the evolution from the system's initial conditions typically exhibits a separation of scales behavior. An example is the modeling of wild fires where small-scale phenomena must account for the turbulent nature of fire while large-scale phenomena exhibit coherent structures that mathematical operators such as the Laplacian may represent with satisfactory accuracy. In structural dynamics, this certainly applies to the phenomena by which energy is dissipated in a structure. For example, the Coulomb damping model provides a deterministic, large-scale description while the phenomenological behavior is highly stochastic and represented by the so-called "stick and slip" at the microscopic level. Generally, statistical models explain these behaviors by coupling mean-field theories to large deviation principles that characterize the most probable states of the system.

This brings us to our first point. The total predictability that may be expected from a particular model depends on the purpose intended for the model. The traditional approach for model validation ("My model is valid because it reproduces my test data with acceptable accuracy…") may be irrelevant when it comes to analyzing statistically-accurate models or phenomenological models that do not necessarily provide deterministic outputs.

The methodology proposed here focuses on the validation of statistically-accurate models as opposed to deterministic models. This focus arises because we believe that the environmental variability and the sources of uncertainty in manufacturing tolerances and assembly procedures must be accounted for to fully capture the whole spectrum of behavior of the systems analyzed (from nominal response to catastrophic failure). Another reason is that the phenomena being studied are too complicated to be modelled in a deterministic manner. Nevertheless, our paradigm is also demonstrated when applied to models that could be qualified as "physically-accurate" because they attempt to capture a particular, deterministic behavior with high fidelity [3]. A second important point is that the concept of model validation should be strongly coupled to the quantification of uncertainty, a relationship that has generally been overlooked by the conventional finite element model updating technology. This relationship is further developed in Section 6.

3.2 Current Trends

It is clear that both public and private sources of funding for research and development in the United States emphasize the new, "soft" technologies to the detriment of hard sciences. Analyzing the priorities at the turn of the century of agencies such as, for example, the NSF (National Science Foundation) and DARPA (Defense Advanced Research Projects for the Army) shows that the vast majority of project funded are in the following areas:

1) **Genetics**;
2) **Information technology**;
3) **Computing**;
4) **Nano-structures**.

There is no reason to believe that this trend will not become even stronger in the coming years, making it critical for professionals in hard sciences and engineering disciplines to seek new opportunities. In light of this, what trademarks make a particular project attractive to a funding agency? What are the current trends in computational sciences? Here, we identify eight such trends that, we believe, characterize recent advancements in hard and soft sciences alike:

1) **The coupling of different models**. To study complex phenomena, several models are developed that must be coupled together. For example, global climate predictions must represent the coupling between atmospheric models, ocean models and ice models. This generally yields to important computational and implementation challenges.

2) **The development of broadband models**. Models are increasingly "broadband," seeking to simulate an experiment over different time scales (from a few nano-seconds to a few minutes or a century in the case of civil infrastructure), frequency scales (from a few Hertz to a few MHz) and energy scales (from a few Watts to a few GeV).

3) **The accurate representation of the geometry**. With the availability of ever-increasing computational power, smaller discretizations are sought after to provide a good representation of the geometry of the system being analyzed. This may lead to very large computational models where the small-scale and large-scale dynamics are coupled.

4) **The propagation of uncertainty**. Stochastic models must enable the propagation of uncertainty during the forward calculations. Solving inverse problems in the presence of uncertainty is, to a great extent, an issue of open research that we address briefly in Section 6.

5) **Combining data with models**. Increasingly, measured initial conditions, measured boundary conditions or experimental data sets of other nature are combined with the models to improve their representation of a particular, hard-to-model component or to improve their correlation with test data. This is generally referred to as "parameter tuning" in most scientific fields. In structural dynamics, this has been the subject of considerable literature in the past years of which the research in model updating [4-5], damage detection [6] or component mode synthesis [7] can be cited as examples.

6) **Developing statistical approximations to expensive computer runs**. Polynomial fits, neural networks, statistical correlation analyses, etc., are attractive alternatives to computational models, a procedure here referred to as the substitution of a "meta-model." There now is an increasing focus on developing meta-models that are statistically accurate and that can be used not only for interpolating and extrapolating the system's response but also for assessing the information content of a given combination of input variables.

7) **Assessing the distribution of unlikely events**. For reliability and safety assessment, it is of paramount importance to estimate the "tails" of the distribution of a simulation output. Methods for reliability analysis are becoming commonly available but their application to large-dimensional, broadband, coupled-physics models raises new issues such as efficient sampling and fast probability integration.

8) **The estimation of ensemble properties**. Case-by-case comparison of data sets tends to be replaced with ensemble comparisons. Without ensemble averaging, scientific theories such as quantum mechanics would simply not exist. It also enables the estimation of the information content of a particular model using adequate probabilities. An illustration of this procedure is the area known as "experimental design" [8].

An example that clearly integrates many of these trends is the modeling of protein forming in computational genetics. It is believed that the interaction between individual molecules can be modelled with sufficient accuracy using classical Newtonian mechanics. This allows analysts to derive the equations of motion analytically with the major drawback of requiring the analysis of very large nonlinear models (10 to 100 million degrees of freedom). It is reported in the literature that the time scale required to capture the first stretching mode of a protein and the corresponding infra-red emission is in the order of 10^{-12} second while the time scale required to capture the shape of the final protein is equal to 0.1 to a few seconds [9].

3.3 What Does it Take to be Predictive?

Even if analyses of this magnitude can be performed on today's most powerful super-computers, the central question remains: What does it take to be predictive? The five elements generally mentioned as being critical when it comes to assessing the predictive accuracy of a model are:

1) **The geometry**;
2) **The physics**;
3) **The sources of uncertainty**;
4) **The model sensitivities**;
5) **The outcome of the model**.

Approximating the geometry and the physics remains an issue of importance in many scientific fields such as wild fire modeling, traffic modeling or global climate prediction. In structural dynamics however, the capabilities are generally available to represent any geometry at any precision level. Similarly, the physics of the systems dealt with is well described, at least at the continuum level, by the equations of solid mechanics and fluid dynamics. Therefore, our discussion in Section 6 will focus on other aspects even if it is acknowledged that significant research efforts are currently being spent in areas such as multi-scale, high-fidelity material modeling. Modeling uncertainty and calculating the model's sensitivities (or estimating the statistical correlation of an output $\mathbf{y}_j$ to an input $\mathbf{p}_i$) may offer significant computational challenges when nonlinear, stochastic models are involved. Similarly, defining the outcome of a model assumes that its purpose can be assessed by adequate features and metrics. Analysts dealing with complex numerical simulations that generate several Giga-bytes of output may be overwhelmed by the amount of data produced. Data interrogation, data compression and pattern recognition tools then become key components of the analysis. These issues are further discussed in Section 6 for nonlinear, stochastic structural dynamics.

4. Structural Dynamics

The purpose of this Section is to specialize the discussion to the particular field of structural dynamics. Trends in modeling and testing are briefly discussed after which we illustrate the current limitations of our modeling capabilities with an example. This points to the need for systematic model validation strategies as outlined in Section 6. Finally, the future of structural dynamics and its impact on test-analysis correlation and inverse problem solving is briefly discussed.

4.1 Testing Versus Modeling

The main reason why numerical models have become so popular is because it is much less expensive to use computational time than it is to run a sophisticated experiment. Many practical situations also occur where the phenomenon of interest can not be measured directly. For example, this is the case with large space antennas developed for observation and communication purposes that do not withstand their own weight in an environment of 1-g of gravity. Hence, the scientific community has turned to numerical models that can be parametrized and used to study a wide variety of situations.

This argument has been reinforced in recent years by the increasing efficiency of processors, the greater availability of memory, the breakthrough of object-oriented data structures together with the growing popularity of parallel processing whether it involves computers with massively parallel architectures or networks of single-CPU workstations. Interestingly enough, the miniaturisation of CPU's and their greater efficiency have influenced greatly testing procedures, making it possible to instrument structures with hundreds of transducers. Powerful data analysis and friendly computer graphics are also a driving force behind the development of non-intrusive, optical measurement systems such as holography and laser vibrometry. These technological breakthroughs are not without major consequences on the way engineers are analyzing structural systems and on their conception of test-analysis correlation and inverse problem solving.

An illustration of this evolution is the rapid development of modeling procedures for nonlinear dynamics. It is reasonable to foresee that the bottleneck of computing power will be removed in the near future, at least when it comes to engineering applications.[4] Consequently, research and development efforts in recent years have been mostly focused on improving the representation of the geometry and the physics. Examples are the derivation of small-scale, statistical models for contact dynamics; the implementation of high-fidelity, nonlinear material models; or the efforts to expand our current modeling capabilities to the high frequency range for predictive acoustics. In spite of these undeniable advances, very rarely have the issues of uncertainty quantification and predictability been raised. Nevertheless, they are central questions when it comes to assessing whether a numerical simulation is capable of reproducing with acceptable accuracy the experiment it is supposed to replace.

4.2 How Complex Can it Get?

An example of complex structural system is now discussed. The sub-components in a modern weapon system comprise over 6,000 parts most of which contribute to the non-structural mass and dynamics. Modeling this system down to the very details of the electronics components is critical for performance and reliability assessments where, for example, it is verified the acceleration and stress levels do not jeopardize the system's survivability. This forces analysts to represent the nonlinear dynamics of different joints such as bolts, welds, threads, compression pads, tapered joints, etc. This is a challenging task because it involves a good understanding and high-fidelity modeling of the energy dissipation mechanisms for each of these scenarios.

The point of this illustration is that, no matter how powerful computers become, there will always be some degree of uncertainty in the numerical models due to unknown interfaces, unknown physics, environmental

[4] The ASCI platforms "BlueMountain" and "Red" at LANL and SNL, respectively, routinely perform over 3 Teraflops distributed over several thousand computational nodes. This power may not yet enable high-energy physics simulations with enough accuracy but it is considered sufficient for most engineering applications. For reference, see: www.sgi.com/newsroom/press_releases/2000/may/blue_mountain.html.

variability, parameter and assembly uncertainty, idealization errors, discretization errors, numerical errors, etc. Increased computational power allows to bound some of these sources of uncertainty (such as discretization and numerical errors), but not all of them can be reduced to desirable levels. Because the trend of replacing expensive laboratory or field experiments with numerical simulations is not going to change, systematic model validation strategies are needed.

Note that many systems dealt with in industries and communities other than the U.S. national laboratories share similar characteristics: distribution of sub-systems and components; interface dynamics; multi-scale behavior; etc. Representing the dynamics of an automobile door and the interaction between the frame and the window, for example, is quite challenging especially when it comes to acoustic predictions.

4.3 Speculative Outlook

When analyzing the dynamic response of a complex system using the FE method, it is not acceptable to neglect the contribution of an important component, joint or interface. In the past, neglected dynamics were accounted for by tuning parameters in the model to agree with the experimental data. For example, the damping (modal or other) was determined "ad hoc" using test data obtained from testing the fully assembled system. Then, the identified damping properties were added to the model to improve its predictive accuracy.

At present, some of the full-scale testing capabilities which formerly existed at the U.S. national laboratories and many other facilities in the automotive, aerospace and civil engineering communities are no longer functional. Therefore, it is no longer possible to reconcile a model with experimental data for all environments. In the future, models will be constructed with limited use of these expensive, full-scale test data sets. In addition, it is our opinion that structural dynamics in the 21st century will become increasingly:

1) **Nonlinear**;
2) **Non-structural**;
3) **Non-modal**;
4) **High bandwidth**;
5) **Multi-physics**.

In these conditions, can the concept of FE model updating that has been developed for linear, modal dynamics be generalized? Is FE model updating the correct answer to model validation? What "features" other than the conventional mode shapes and resonant frequencies can be extracted from the data to characterize the response of a nonlinear system? How to quantify the total uncertainty of an experiment? How to propagate the parametric uncertainty of a numerical simulations? These are some of the questions that we try to address in the remainder.

5. Finite Element Model Updating

The technology available for the optimisation of nonlinear dynamic systems based on test-analysis correlation is briefly reviewed. We start by presenting the conventional approach to FE model updating. In particular, those elements that could make it possible to apply the available technology to nonlinear systems are discussed. Then, the approach based on optimal error control is summarized. It proposes a different formulation of the inverse problem that is better suited to the optimization of both parametric and non-parametric models for nonlinear dynamics.

5.1 Conventional Approach

Finite element model updating for linear and nonlinear dynamics generally consists in formulating criteria for measuring the correlation between test data and FE results. If we consider, first, any type and source of nonlinearity and, second, both parametric and non-parametric updating, very few techniques are available from the published literature that can handle these constraints.[5] For an illustration of the lack of techniques relevant to the nonlinear world, the reader is invited to review from References [4-5] the state-of-the-art in model updating technology. Among the earliest and most promising work in test-analysis correlation for nonlinear dynamics, we cite the work by Hasselman et al. [10] and Dippery et al. [11].

Generally, parametric optimization is achieved by minimizing a "distance" between experimental data and numerical predictions, whether this distance is evaluated in the time or frequency domain. The optimization problem is formulated as the minimization of the cost function shown in equation (1) where the first contribution represents the metric used for test-analysis correlation and the second serves the purpose of regularization

$$\min_{\{\delta \mathbf{p}\}} \sum_{\mathbf{j=1 \cdots N_{data}}} \{\mathbf{R_j}\}^* \left[\mathbf{S_{RR_j}}\right]^{-1} \{\mathbf{R_j}\} + \{\delta \mathbf{p}\}^T \left[\mathbf{S_{pp}}\right]^{-1} \{\delta \mathbf{p}\} \qquad (1)$$

[5] Techniques are available from the system identification literature for identifying nonlinear responses and fitting parametric models. An example is the application of Voltera kernels. However, in the overwhelming majority of cases, the type of nonlinearity and the corresponding mathematical model must be known ahead of time. This is not practical when dealing with complex engineering applications. Similarly, the reason for emphasizing both parametric and non-parametric identifications is because all sources of uncertainty and modeling errors may not be known, in which case a non-parametric technique (a.k.a. total uncertainty, residual approach, etc.) is the only possible alternative.

Parameters **{p}** in equation (1) represent the subset of design variables selected to be optimized. The model's input-output relationship is denoted by

$$\mathbf{y(t) = M(p, t)} \tag{2}$$

where **y(t)** represents the desired set of outputs (essentially, time-domain responses) from which the features $\{\mathbf{R_j}\}$ are estimated. The model defined in equation (2) can have an arbitrary form (modal, linear, nonlinear, implicit, explicit, etc.) and an arbitrary purpose (high-fidelity prediction, phenomenological extrapolation, reliability assessment, etc.). This is somewhat irrelevant to the discussion although the large majority of FE model updating techniques assume a linear, modal simulation. The main three ingredients of FE model updating are:

1) **Features**. Features $\{\mathbf{R_j}\}$ are the time-domain or frequency-domain quantities defined for the purpose of test-analysis correlation. For linear dynamics, the simplest and most popular of all are the resonant frequencies, mode shapes and modal damping ratios [12]. Two other important features that we cite for completeness are the force and hybrid modal residues defined in References [13] and [14], respectively. Feature extraction for nonlinear experiments is addressed in Section 5.2.

2) **Metrics**. The metric is defined as the norm used for comparing the features $\{\mathbf{R_j}\}$ extracted from the test and analysis data sets. The weighted Euclidean norm adopted in equation (1) is a popular choice because it facilitates algebraic derivations. This choice is generally not an issue because all norms are equivalent in finite dimensional spaces. However, in the context of model validation for nonlinear, stochastic simulations, such metrics become statistical hypothesis tests.

3) **Constraints**. Constraints such as $\mathbf{p_{min} < p < p_{max}}$ are generally added to the formulation to filter out local minima that would not be acceptable from a physical standpoint. Accounting for constraints requires efficient optimization solvers that may not always be readily available.

4) **Optimization**. Many optimization solvers can be implemented depending on the availability of gradient and Hessian information [15]. Global search methods such as genetic algorithms are sometimes used with great success but their computational burden makes them impractical when dealing with real-world applications.

5) **Weighting**. Weighting matrices in equation (1) are generally kept constant and diagonal for computational efficiency. They can also be defined as covariance matrices which then formulates a Bayesian correction procedure, as shown in Reference [16]. The only real difficulty is to track the evolution of the covariance coefficients as parameters in the model are adjusted.

6) **Spatial Incompleteness**. The number-one issue in FE model updating is the mismatch between sensor locations and degrees of freedom of the model. In the linear domain, modal expansion techniques have been proposed to expand the identified mode shapes [17-18]. Model reduction is an alternative that reduces the FE matrices and force vectors down to the subset of measurement locations. Many techniques have been published in the past three decades to achieve this objective, a recent review of which can be found in Reference [7]. Nonlinear model reduction is being studied but rarely in application to structural dynamics. Attempts have recently been made to assess the efficiency of nonlinear model reduction in the context of nonlinear FE model updating [19-20]. These results are preliminary and we believe that more research is required to demonstrate this concept. In addition, nonlinear model reduction techniques are generally based on modal data which requires that the equations of motion be linearized. This is a severe limitation when it comes to analyzing systems with discontinuous nonlinearities such as contact. Unfortunately, the same argument applies to modal expansion.

5.2 Feature Extraction

The overwhelming majority of FE model updating techniques are restricted to linear models and modal data. To analyze nonlinear systems, non-modal features must be defined because the notion a "representative" subspace spanned by a few low-frequency mode shapes is replaced by time-varying, state-space manifolds.

To date, very little work is available on the updating of nonlinear FE models. Among the earliest approaches that have been applied with success to realistic testbeds, we cite References [10-11,21]. These methods conform to the general framework presented previously and they have in common that the features $\{\mathbf{R_j}\}$ are simply defined as the difference between time-domain responses (such as acceleration, strain or pressure) measured and simulated by the numerical model.

Instead of comparing explicitly, say, the acceleration data, the approaches presented in References [21-22] gather these time series at multiple output locations into a matrix that can be analyzed using the Singular Value Decomposition (SVD). In addition to filtering out the measurement noise and unessential dynamics, this procedure generates time-varying, Karhunen-Loeve basis functions that span the nonlinear manifolds the same way mode shapes span an invariant subspace. Then, the features **{R_j}** are defined as the difference between test and analysis basis functions (left singular vectors), energy contributions (singular values) and time-varying amplification factors (right singular vectors). Application examples documented in Reference [21] demonstrate that this analysis technique is very powerful for understanding the nonlinear dynamics of a complex structure.

5.3 Optimal Error Control

With the conventional approach for solving inverse problems, a parametric optimization is formulated by defining a time-domain feature and by solving for the optimum solution **{p^*}** that minimizes the cost function shown in equation (1). Obviously, this procedure must be repeated over several time windows **[t_i;$t_{(i+1)}$]** if the design variables **{p}** are time-varying quantities. However, nothing in the formulation of the inverse problem (1) enforces continuity between the solution fields obtained from models optimized within the i^{th} and $(i+1)^{th}$ time windows. This issue is fundamental because the sequence of optimized models will yields discontinuous acceleration, velocity and displacement fields which contradicts the laws of mechanics for the class of problems investigated here.

The only solution currently available is to re-formulate the inverse problem as a constrained optimization where the continuity of the solution field is enforced explicitly. This strategy is based on the theory of optimal control and it relies on the resolution of multiple two-point Boundary Value Problems (BVP) [11,23]. When satisfactory solutions of the two-point BVP's are obtained, the adjusted numerical model is guaranteed to match the measured data at the beginning and at the end of the time window considered. A typical implementation would feature the resolution of a two-point BVP each time a set of features **{R_j}** is estimated for a given combination of design variables **{p}**. Since this procedure is embedded within an optimization solver, multiple two-point BVP's must be solved for. Unfortunately, the impact on the computational requirement is enormous and practical applications exceeding a few degrees of freedom in complexity currently remain out-of-reach.

6. Model Validation

We have seen that, for a wide variety of applications, techniques based on linear dynamics and modal superposition are likely to fail. Hence, it is critical to validate numerical models by correlating transient test data rather than steady-state, modal data. However, formulating correctly the inverse problem in this case requires to solve multiple two-point BVP's that exhibit prohibitive computational requirements, as explained previously. Throughout Section 6, the relationship between conventional FE model updating and the "big picture" of uncertainty quantification and model validation is explored and specific technological issues are discussed.

6.1 The Big Picture

Our "philosophy" is to replace the minimization (1) by a methodology where error surfaces are generated from the resolution of a large numbers of forward, stochastic analyses, then, optimized to identify the source of modeling error [24]. It is the alternative to the correct yet computationally impractical formulation discussed in Section 5.3. Figure 1 provides an overview of model validation for nonlinear, stochastic dynamics.

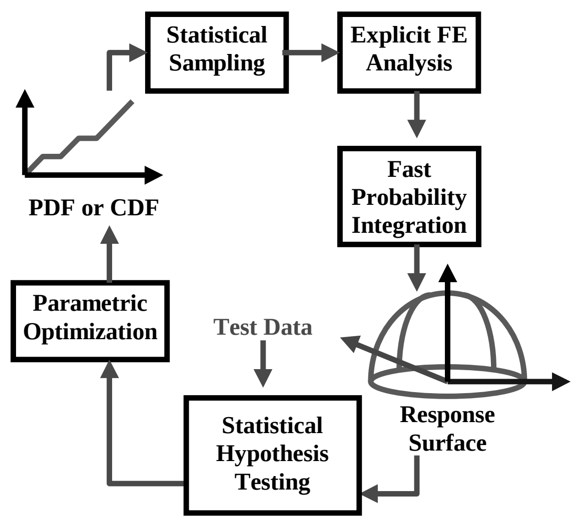

Figure 1. Flow chart of model validation.

According to Figure 1, optimization parameters and random variables are first defined. Multiple FE solutions and multi-dimensional error surfaces are generated from statistical sampling. Error surfaces provide a metric for test-analysis correlation and model updating. The metrics adopted may be defined as statistical hypothesis tests used for assessing the consistency between a probabilistic FE simulation and a series of test data sets. The "statistically most accurate" model is then sought after through the optimization of its design parameters. Where these consist of random variables, the procedure must either search for the most likely parameters (case where distributions are known) or optimize the statistics (case where distributions are somewhat unknown). Rather than comparing the response output, the ability of a probabilistic model to reproduce test data must be assessed using the response's probability or cumulative density functions.

Besides having to account for uncertain inputs, imperfect material characterization and modeling errors during a design cycle, the other reason for this approach is to recast model updating as a problem of hypothesis testing. When the predictive quality of a model is assessed, we believe that three fundamental questions must be answered:

1) **Are the experiments and simulations consistent statistically speaking**?

2) **What is the degree of confidence associated with the first answer**?

3) **If additional data sets are available, by how much does the confidence increase**?

Hypothesis testing permits to answer these questions. The difficulty however is to assess the minimum amount of data necessary to formulate a meaningful test and to implement such a test for large-scale, numerical simulations. Although hypothesis testing is well-known, very little literature is available on the subject of "population versus population" testing. This makes the whole procedure a non-trivial task and a matter of open research to a great extent.

6.2 Model Updating vs. Model Validation

We would like to emphasize that model validation is a broader concept than model updating. A numerical simulation is not necessarily validated after the output has been compared to test data and the model has been updated. Instead, it is generally agreed upon that new, well-thought strategies must be established for model validation. They integrate tools such as component testing, full-scale testing, test-analysis correlation, statistical analysis and FE model updating. Figure 2 illustrates the implementation of model validation where errors caused by our imperfect knowledge of "separable" physics (that is, effects that can be decoupled from each other) are identified first. Then, the sources of variability and modeling errors that may result from the successive steps of system integration are identified and corrected. At the separable physics or continuum levels, phenomena are generally complex but dedicated and well-controlled testing procedures can be defined. At the sub-assembly or full-scale levels, testing is difficult and variability may be a concern but few unknowns remain to be inferred from test data.

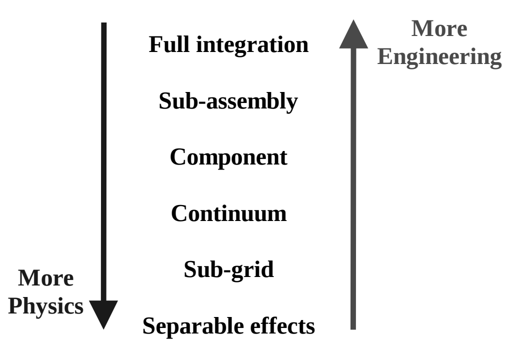

Figure 2. Successive levels of model validation for a complex experiment.

In addition to recognizing that a model must be gradually validated, great attention should also be paid to the operating conditions and the model's purpose. Clearly, two different experiments and probably two different models must be developed when the same component is subjected to random vibrations or shock response. The purpose of a model is also of paramount importance because it dictates the features and metrics on which the validation should focus. As a result, model validation must be thought of in terms of a matrix of experiments rather than a single test-analysis correlation study. An example is provided in Figure 3 where the coupling between models and loads applied is illustrated. To be complete, a third axis that would represent the model's purpose should be added.

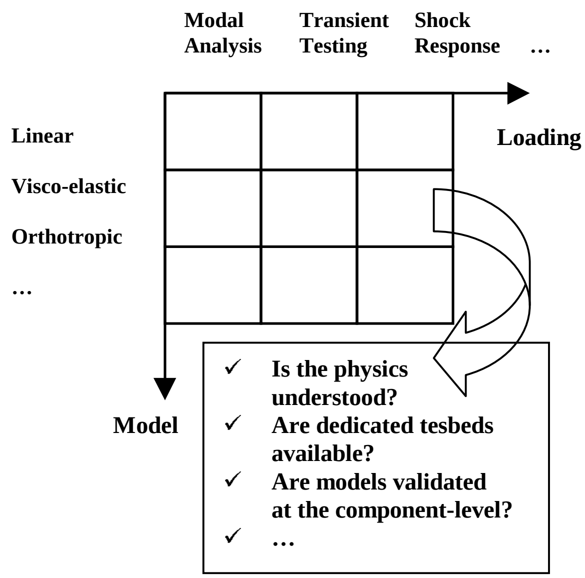

Figure 3. Matrix of model validation experiments.

An example of practical implementation of this paradigm is the validation of complex engineering simulations performed at LANL for the ASCI program. The application illustrated in Figure 4 represents the highly transient response of a threaded joint assembly due to explosive loading. Prior to assessing the validity at the full-scale level, phenomenological testing is performed to identify the characteristics of an aluminum-to-steel contact pair subjected to nonlinear vibrations. Then, a controlled experiment is designed to validate the model of a hyper-elastic material when a shock produces high-rate deformations in the material. Finally, these various components are integrated together. The resulting nonlinear and explicit FE model features more than 10 million degrees of freedom. When running on an ASCI platform with 700 dedicated processors, one hour of CPU time is required to simulate 10^{-3} second of response. Full-scale, explosive testing is performed and model validation is used to identify specific joint properties as well as the degree of variability of the assembly.

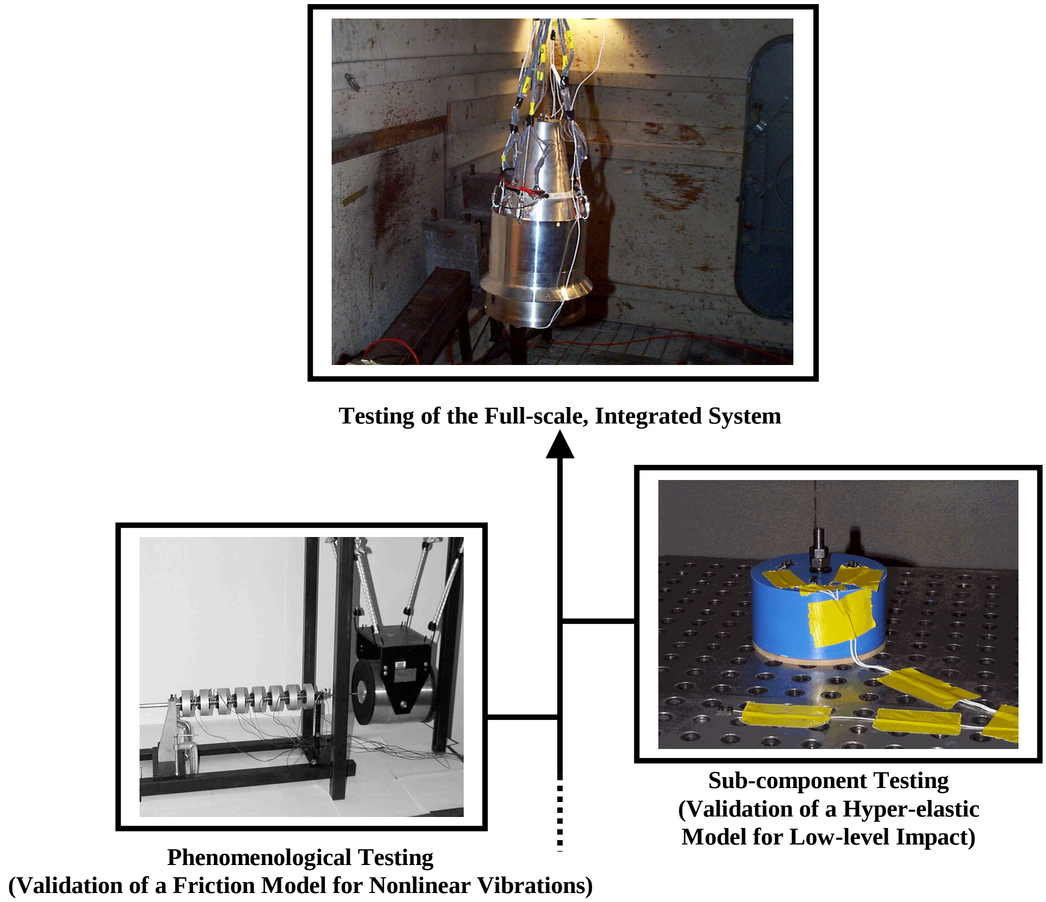

Figure 4. Implementation of model validation for the ASCI program at LANL.

The ultimate task of verifying that predictions of the optimized model are correct remains a challenging one. This is nothing less but the old mathematical dilemma between interpolation and extrapolation. Our opinion of this issue is that model validation does not exist. There is only model “invalidation” as demonstrated by Pearson’s work on hypothesis testing [25], that is, a model may be considered correct as long as it can not be proved wrong. Practically, this means that:

1) **Data sets not used during the validation step are required to assess the predictive quality of a model**.

2) **Probabilities must be assigned to each model developed to reflect the degree of confidence (or lack of confidence) in their predictions**.

6.3 Orientations of the Research

We have seen that modal-based criteria form the vast majority of FE model updating techniques. These become rapidly obsolete when systems are subjected to high-frequency excitation, when variability is an issue of concern or when the dynamics of interest are strongly nonlinear. In the remainder, five issues are discussed that are critical to the success of model updating and model validation for nonlinear dynamics.

1) **Uncertainty quantification**. The success of any model validation depends on the ability to quantify uncertainty. The current approach in statistical sciences is to analyze the error of the model output. This is not efficient for identifying the sources of discrepancy between test and analysis results. Instead, the uncertainty should be built at the beginning of the analysis, then propagated through the forward resolution. One potential approach is Bayes inference [26] where the posterior probability, that is, the probability of the model **{p}** given data **{y}** is obtained as

$$\mathbf{P}(\mathbf{p} \mid \mathbf{y}) = \frac{\mathbf{P}(\mathbf{y} \mid \mathbf{p})\mathbf{P}(\mathbf{p})}{\mathbf{P}(\mathbf{y})} \tag{3}$$

What is therefore important is not necessarily that the correlated models reproduce the responses measured during a single test but that they predict the response levels with the same probability of occurrence as the one inferred from test data.

2) **Sampling and fast probability integration**. The notions discussed here rely strongly on the capability to propagate uncertainty and/or variability throughout an analysis. For large-scale applications featuring nonlinear models, Monte Carlo simulations remain computationally too

inefficient when it comes to predicting unlikely or catastrophic events, which is one of the main reasons for carrying out an analysis. Stochastic finite element techniques [27] and fast probability integration methods [28] must therefore be developed and interfaced with engineering codes. Accelerated sampling methods such as the Latin Hypercube Sampling are efficient alternatives [29].

3) **Generation of meta-models**. Efficient numerical optimization requires that the objective functions be obtained at low computational cost. Therefore, meta-models or fast running models must be generated to replace the expensive, large-scale simulations. One difficulty of fitting meta-models is efficient sampling, that is, the generation of sufficient information in regions where the feature's joint probability density function is maximum. This particular issue is the focus of recent advances in the statistics community [30].

   The second direction of open research is the implementation of probabilistic meta-models when the objective of model validation is to account for sources of variability in the experiment and the numerical model. Stochastic processes can also be included to propagate other sources of discrepancy between test and analysis data such as numerical and truncation errors or to bound the experiment's total uncertainty. This procedure, well-known in the geo-physics community, is progressively being tested and applied in structural dynamics [8].

4) **Feature extraction**. Large computer simulations tend to generate enormous amounts of output that must be synthesized into a small number of indicators for the analysis. This step is referred to as data reduction or feature extraction [31]. These features are typically used to define the test-analysis correlation metrics optimized to improve the predictive accuracy of the model. The main issue in feature extraction is to define indicators that provide meaningful insight regarding the ability of the model to capture the dynamics investigated. Features that we are using to analyze nonlinear, transient data sets include: the RMS error of time series; the principal component decomposition; the shock response spectrum; ARX and ARMA-based features; the power spectral density (Fourier transform of the auto-correlation function of a signal); higher-order statistical moments; and probability density functions.

5) **Statistical hypothesis testing**. One of the open research issues that this work has identified is the problem of establishing a correlation between multiple data sets. By this we mean "assessing the degree to which two populations are consistent with each other." Such statistical consistency can be assessed using the Mahalanobis distance and a standard, multivariate Hotelling's T^2 test. This statistics, however, can only compare the mean of two distributions. One of the only possibility available for testing both mean and variance is to calculate Kullback-Leibler's relative entropy defined as the expected value of the ratio between the PDF's of the two populations. These statistics are attractive because they are independent of the parent distribution.

   The computational requirement associated with this procedure may become very important because the probability distribution of each feature considered for test-analysis correlation must be assessed for each candidate design evaluated during the optimization. This, however, is the only possibility to guaranty at a given confidence level that the numerical simulation is validated in the context of uncertainty propagation.

7. Conclusion

A general framework is discussed for validating numerical models for nonlinear, transient dynamics. To bypass difficulties identified when applying test-analysis correlation methods to nonlinear data sets, inverse problems are replaced with multiple forward, stochastic problems. After a statistical metric has been defined for comparing test and analysis data, response surfaces are generated that can be used for assessing in a probabilistic sense the quality of a particular simulation with respect to "reference" or test data and for optimizing the model's design parameters to improve its predictive quality. Current directions of research are stated throughout this publication. Several experiments have been conducted at Los Alamos National Laboratory in support of our ASCI and code validation programs to validate the models of complex engineering simulations. Several illustrations of this methodology and preliminary results can be obtained from References [3,24].

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